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Influence of Spin-Orbit Coupling on Electronic Transitions in Organic and Inorganic Systems

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Spin-orbit coupling (SOC) plays a critical role in modulating the efficiency and dynamics of electronic transitions in both organic and inorganic systems. In organic-inorganic heterojunctions, SOC enhances electron transfer and spin-flip processes, as demonstrated in the ZnPc/MoS_2 heterojunction, where SOC enables fast electron relaxation pathways and spin transitions, significantly improving device performance in photovoltaic and photocatalytic applications.[1] Similarly, purely organic systems typically exhibit weak SOC; however, the introduction of heavy atoms or molecular flexibility, such as in the thianthrene-pyrimidine based compound, dramatically boosts SOC. This leads to enhanced intersystem crossing rates and efficient room-temperature phosphorescence, as evidenced by the development of high-efficiency organic light-emitting diodes (OLEDs).[2] Furthermore, the geometry of molecular oxygen complexes with nearby atoms significantly influences the magnitude of SOC, with specific configurations enhancing SOC through asymmetrical orbital interactions.[3] These findings illustrate the central importance of SOC in governing electron dynamics across a range of organic and inorganic systems, offering promising avenues for designing more efficient electronic and photonic devices.

References

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2. Qiu, W.; Cai, X.; Chen, Z.; Wei, X.; Li, M.; Gu, Q.; Peng, X.; Xie, W.; Jiao, Y.; Gan, Y.; Liu, W.; Su, S.-J. A "Flexible" Purely Organic Molecule Exhibiting Strong Spin–Orbital Coupling: Toward Nondoped Room-Temperature Phosphorescence OLEDs. *J. Phys. Chem. Lett.* **2022**, *13* (22), 4971–4980. https://doi.org/10.1021/acs.jpclett.2c01205.
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